A VARIATIONAL APPROACH TO THE GROUND STATE ENERGY OF THE ELECTRON GAS

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CHAPTER I

INTRODUCTION

A standard procedure for obtaining an upper bound on the ground

state energy and an approximation to the ground state wave function

Ψ for a system is to write the energy in terms of the wave function

and then minimize it with respect to variation of the wave function.

This is the Rayleigh-Ritz variational method. We shall present a

means of using this procedure for an electron gas, using a trial

wave function of the form $De^{A/2}$, where D is the wave function for

an ideal gas of spin 1/2 particles. We shall specialize to the form

where A is real and is given by

$$A \simeq -\sum_{i<j} u(r_{ij}).$$
(1.1)

That this is a reasonable assumption is indicated by the fact that

the system under consideration differs from an ideal gas only by

virtue of the presence of Coulomb forces. Such two-body forces

depend only on the distance of separation between the particles.

Some information about the form of $u(r)$ is already available since

the wave function must obey certain boundary conditions in order to

properly describe the system under consideration. Specifically, as

r becomes infinitely large, $u(r)$ must vanish, and, the work of Dunn[1,12]

indicates that $u(0)$ is a constant, which allows tunneling effects to

be observed. The work of Dunn,[1,12] and others,[2] further indicates

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that the function $u(r)$ galls off as $(r)^{-1}$ in the large r limit. A simple functional form for $u(r)$ which obeys these conditions is given by,[†]

$$u(r) = \frac{a}{r}(1-e^{-br}),$$ (1.2)

where a and b are unknown parameters to be determined. If this form of $u(r)$ is adopted, one can express the wave function, and, consequently, also the energy for the system, as a function of the two constants a and b. This fact leads to the simple variational procedure later employed in this thesis.

The Hamiltonian operator $\mathcal{H}$ for an electron gas can be written as

$$\mathcal{H} = -\frac{\hbar^2}{2m}\Delta^2 + V(\vec{r}_1\ldots\vec{r}_N)$$ (1.3)

where

$$\Delta^2 = \sum_{a=1}^{N}\nabla_a^2 = \sum_{a=1}^{N}\sum_{\ell=1}^{3}\frac{\partial^2}{\partial x_j^{\ell 2}}$$ (1.4)

and $V(\vec{r}_1\ldots\vec{r}_N)$ represents the Coulomb potential. The expectation value of the energy, $\langle E\rangle$, is then

$$\langle E\rangle = \frac{\int\ldots\int\Psi^*[-\frac{\hbar^2}{2m}\Delta^2+V]\Psi d\vec{r}_1\ldots d\vec{r}_N}{\int\ldots\int\Psi^*\Psi d\vec{r}_1\ldots d\vec{r}_N}.$$ (1.5)

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[*]Strictly speaking, $u(r)$ is defined by

$$u(r) \equiv 4\pi ab^2{\sum_{\vec{k}}}' \frac{e^{i\vec{k}\cdot\vec{r}}}{k^2(k^2+b^2)},$$

where the prime on the summation sign indicates that the k = 0 term is to be excluded from the summation. However, for our purposes, Eq.(1.2) is valid as long as the quantity $g(r)-1$ is used in the kinetic energy expressions. This matter is discussed in detail in Chapter III.

In Chapters II and III it is shown that Eq.(1.5) can be written in terms of integrals involving the radial distribution function $g(r)$. This function is defined as

$$g(r_{12}) = \frac{\Omega^2 \int \ldots \int \Psi^* \Psi d\vec{r}_3 \ldots d\vec{r}_N}{\int \ldots \int \Psi^* \Psi d\vec{r}_1 \ldots d\vec{r}_N}, \qquad (1.6)$$

where Ω is the volume of the system. Noting that the product D^*D is symmetric, we approximate it by writing

$$D^*D \cong \exp\left(-\sum_{i<j} \phi(r_{ij})\right), \qquad (1.7)$$

where the function $\phi(r)$ has already been determined from the ideal gas calculations of Lado and Dunn.[3] Therefore $\Psi^*\Psi$ may be written as

$$\Psi^*\Psi \cong D^*D\exp\left(-\sum_{i<j} u(r_{ij})\right) = \exp\left(-\sum_{i<j} \theta(r_{ij})\right), \qquad (1.8)$$

where

$$\theta(r) \equiv \phi(r)+u(r).$$

Since the product $\Psi^*\Psi$ can be expressed in the form $\exp\left(-\sum_{i<j} \theta(r_{ij})\right)$, we are able to employ several powerful techniques for evaluating $g(r)$. Among the most useful of these are Lado's pertubation formula[4,11] and the Percus-Yevick integral equation.[5] In this work the latter method is employed in the region of metallic densities, while the former is used for high densities.

CHAPTER II

DERIVATION OF THE BASIC EQUATION

In the introduction the expectation value of the energy was defined in Eq.(1.5) as

$$<E> = \frac{-\frac{\hbar^2}{2m}\int\Psi^*\Delta^2\Psi d\tau + \int V\Psi^*\Psi d\tau}{\int\Psi^*\Psi d\tau}, \tag{2.1}$$

where

$$d\tau = d\vec{r}_1 \ldots d\vec{r}_N. \tag{2.2}$$

We must now reduce this expression to a more tractable form in order to apply the variational principle.

First, we will treat the potential energy term given by

$$<P.E.> = \frac{\int\Psi^* V\Psi d\tau}{\int\Psi^*\Psi d\tau}. \tag{2.3}$$

Since $V(r_1 \ldots r_N)$ represents the Coulomb potential, we may define a two-body term $v(r_{ij})$ in the following manner:

$$V(\vec{r}_1 \ldots \vec{r}_N) = \sum_{i<j} v(r_{ij}). \tag{2.4}$$

Using the definition of the radial distribution function $g(r)$, given in Eq.(1.6), we write the potential energy term as

$$<P.E.> = \frac{\rho^2}{2}\int v(r_{12})g(r_{12})dr_1 dr_2$$

$$= \frac{\rho}{2}\stackrel{N}{\int} v(r)g(r)d\vec{r}. \tag{2.5}$$

The function U(r) can be expressed as

$$v(r) = \frac{1}{\Omega} \sum_{\vec{k}}' \nu_k e^{i\vec{k}\cdot\vec{r}}, \qquad 6 \qquad (2.6)$$

where the prime indicates that the k equal to zero term is not included in the summation. Thus

$$\int v(r_{12})d\vec{r}_1 d\vec{r}_2 = \frac{1}{\Omega} \sum_k' \nu_k e^{i\vec{k}\cdot\vec{r}_{12}} d\vec{r}_1 d\vec{r}_2$$

$$\qquad (2.7)$$

$$= \Omega \sum_k' \nu_k \delta(k)\delta(-k) = 0.$$

Therefore

$$\frac{\rho}{2}\int v(r)g(r)d\vec{r} = \frac{\rho}{2}\int v(r)[g(r)-1]d\vec{r}. \qquad (2.8)$$

For the case under consideration, v(r) may be expanded as[7]

$$v(r) = e^2 \left| \frac{1}{r} - \frac{a_0}{L} + \frac{a_1 r^2}{L^3} + \ldots \right|. \qquad (2.9)$$

Thus

$$\frac{\rho}{2}\int v(r)g(r)d\vec{r} = \frac{\rho e^2}{2}\int \left| \frac{1}{r} - \frac{a_0}{L} + \frac{a_1 r^2}{L^3} + \ldots \right| [g(r)-1]d\vec{r}. \qquad (2.10)$$

In the limit as L approaches ∞, we have

$$\frac{\rho}{2}\int v(r)g(r)dr = \frac{\rho e^2}{2}\int [g(r)-1]\frac{1}{r} \, d\vec{r}; \qquad (2.11)$$

and

$$<P.E.> = N \frac{\rho e^2}{2}\int \frac{1}{r}[g(r)-1]d\vec{r}. \qquad (2.12)$$

In order to reduce the kinetic energy term in Eq.(2.1), we first note that integration by parts yields the following relationship:

$$-\int \Psi^* \Delta^2 \Psi d\tau = +\int \Delta\Psi^* \cdot \Delta\Psi d\tau, \qquad (2.13)$$

where the surface terms cancel, due to the boundary conditions imposed on Ψ (see Appendix A). Substituting our form for the wave function, given by

$$\Psi = De^{A/2},\tag{2.14}$$

into Eq.(2.13) we find that

$$-\int \left| D^*\Delta^2 D + D^*\Delta D\cdot\Delta A + \frac{D^*D\Delta^2 A}{2} + \frac{D^*D(\Delta A)^2}{4}\right| e^A d\tau$$

$$\int \left| \Delta D^*\cdot\Delta D + \left(\frac{D\Delta D^*+D^*\Delta D}{2}\right)\cdot\Delta A + \frac{D^*D(\Delta A)^2}{4}\right| e^A d\tau.\tag{2.15}$$

Taking the complex conjugate of Eq.(2.15) and adding shows that

$$\int (\Delta D^*\cdot\Delta D)e^A d\tau = -\int [D^*\Delta^2 D + \Delta(D^*D)\cdot\Delta A$$

$$+ \frac{1}{2}D^*D\Delta^2 A + \frac{1}{2}D^*D(\Delta A)^2]e^A d\tau.\tag{2.16}$$

In arriving at the above result, use was made of the fact that

$$D^*\Delta^2 D = D\Delta^2 D^*.\tag{2.17}$$

To show this, we note (as shown in Appendix C) that

$$\Delta^2 D = \left(-\sum_j \vec{k}_j^2\right)D,\tag{2.18}$$

where the $\vec{k}_j$'s form the complete set of propagation vectors making up D. For the ground state of the system under consideration we will have half the spins "up" and half the spins "down." The summation sign employed in Eq.(2.18) therefore means, that for every value of j, there will be two $\vec{k}_j$'s, one for spin "up" and one for spin "down." Since the $\vec{k}_j$'s are real quantities, it is apparent from Eq.(2.18) that

$$D^*\Delta^2 D = \left(-\sum_j \vec{k}_j^2 D^* D\right) \tag{2.19}$$

and

$$D\Delta^2 D^* = \left(-\sum_j \vec{k}_j^2\right) DD^*. \tag{2.20}$$

Equation (2.19) along with Eq.(2.20) shows that Eq.(2.17) is valid. Substitution of Eq.(2.16) into the right hand side of Eq.(2.15) yields

$$\int \Delta\Psi^* \cdot \Delta\Psi d\tau = \int \left| -D^*\Delta^2 D - \frac{\Delta(D^*D)\cdot\Delta A}{2} \right.$$
$$\left. - \frac{D^*D\Delta^2 A}{2} - \frac{D^*D(\Delta A)^2}{4} \right| e^A d\tau. \tag{2.21}$$

Integrating the second term of Eq.(2.21) by parts gives

$$\int [\Delta(D^*D)\cdot\Delta A] e^A d\tau = -\int D^*D[(\Delta A)^2 + \Delta^2 A] e^A d\tau. \tag{2.22}$$

Substituting Eq.(2.22) into Eq.(2.21) we find that

$$\int \Delta\Psi^* \cdot \Delta\Psi d\tau = \int \left| -D^*\Delta^2 D + \frac{D^*D(\Delta A)^2}{4} \right| e^A d\tau. \tag{2.23}$$

To further simplify Eq.(2.23) we note that Eq.(2.17) may be rewritten as

$$\frac{\hbar^2}{2m}(D^*\Delta^2 D) = \left(-\frac{\hbar^2}{2m}\sum_j k_j^2\right) D^* D, \tag{2.24}$$

where the expression $-\frac{h^2}{2m}\sum_j \vec{k}_j^2$ is just the ideal gas ground state energy, which we shall write as $\frac{3}{5}N\varepsilon_F$, where $\varepsilon_F = \frac{h^2 k_F^2}{2m}$ (see Appendix B). Therefore, using Eq.(2.24) in Eq.(2.23), we see that the kinetic energy may be written as

$$<K.E.> = \frac{\frac{\hbar^2}{2m}\int \Delta\Psi^* \cdot \Delta\Psi d\tau}{\int \Psi^* \Psi d\tau}$$

$$= \frac{3}{5} N\epsilon_F + \frac{\frac{\hbar^2}{8m}\int (\Delta A)^2 \psi^* \psi d\tau}{\int \psi^* \psi d\tau}.$$

(2.25)

The expression $[\Delta A]^2$ is defined as

$$[\Delta A]^2 = \sum_{a=1}^{N} \nabla_a [\sum_{i<j} u(r_{ij})] \cdot \nabla_a [\sum_{\ell<m} u(r_{\ell m})].$$

(2.26)

A brief manipulation shows that

$$[\Delta A]^2 = \sum_{a,i,j}^{N} \nabla_a u(r_{ai}) \cdot \nabla_a u(r_{aj}),$$

(2.27)

where the terms involving $u(0)$ do not contribute, since $u(0)$ is a constant. Substituting Eq.(2.27) into Eq.(2.25) and using the result obtained in Eq.(2.12), we find that the expectation value of the energy may be written as follows:

$$E = \frac{3}{5} N\epsilon_F + \frac{\hbar^2}{8m} \frac{\int\int \left| \sum_{a,i,j} \nabla_a u(r_{ai}) \cdot \nabla_a u(r_{aj}) \right| \psi^* \psi d\tau}{\int \psi^* \psi d\tau}$$

$$+ \frac{N\rho e^2}{2} \int \frac{1}{r} [g(r)-1] d\vec{r}.$$

(2.28)

Equation (2.28) may be written in terms of two-and three-body distribution functions alone, where we define the three-body distribution function as

$$g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \frac{\Omega^3 \int \psi^* \psi d\vec{r}_4 \ldots d\vec{r}_N}{\int \psi^* \psi d\tau}.$$

(2.29)

To this end we can use Eq.(1.8), along with symmetry considerations, to show that

$$\frac{\int\int \left| \sum_{a,i,j} \nabla_a u(r_{ai}) \cdot \nabla_a u(r_{aj}) \right| \psi^* \psi d\tau}{\int \psi^* \psi d\tau}$$

(2.30)

$$= \frac{N(N-1) \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{12}) \psi^* \psi d\tau}{\int \psi^* \psi d\tau} + \frac{N(N-1)(N-2) \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) \psi^* \psi d\tau}{\int \psi^* \psi d\tau}.$$

Using the definition of $g(r)$ as given by Eq.(1.6) along with Eq.(2.29) we see that the right hand side of Eq.(2.30) may be written as

$$N\rho \int \left(\nabla u(r)\right)^2 g(r)\,d\vec{r} + N\rho^2 \int \nabla_1 u(r_{12})\cdot\nabla_1 u(r_{13})g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,d\vec{r}_{12}d\vec{r}_{13}. \qquad (2.31)$$

Using the above result in Eq.(2.28), we find that

$$<E> = \frac{3}{5} N\varepsilon_F + N \frac{\hbar^2\rho}{8m} \int \left(\nabla u(r)\right)^2 g(r)\,d\vec{r}$$

$$+N \frac{\hbar^2\rho^2}{8m}\int \nabla_1 u(r_{12})\cdot\nabla_1 u(r_{13})g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,d\vec{r}_{12}d\vec{r}_{13} \qquad (2.32)$$

$$+N \frac{\rho e^2}{2} \int \frac{1}{r}[g(r)-1]\,d\vec{r}.$$

CHAPTER III

APPLICATION OF APPROXIMATIONS

In Chapter II the energy expression was reduced as far as possible without resorting to some form of approximation. To proceed further, we will employ the random phase approximation[1,13] in the high density region, and the superposition approximation[8,9] for the region of metallic densities.

The Random Phase Approximation

It was shown in Eq.(2.25) that the kinetic energy involved a term containing the expression $(\Delta A)^2$. We wish to apply the random phase approximation to this function in order to reduce it, and consequently, also the expression containing it, to a more easily handled form. In the introduction we saw that the function $u(r)$ could be written as

$$u(r) = \frac{1}{\Omega} \sum_{\vec{k}}{}' \phi(k) e^{i\vec{k}\cdot\vec{r}}. \tag{3.1}$$

Substituting Eq.(3.1) into Eq.(2.27) yields

$$(\Delta A)^2 = \frac{1}{\Omega^2} \sum_{a} \sum_{i,j} \sum_{\vec{m},\vec{k}}{}' (i\vec{k}\phi(k) e^{i\vec{k}\cdot\vec{r}_{ai}}) \cdot (2\vec{m}\phi(m) e^{i\vec{m}\cdot\vec{r}_{aj}}). \tag{3.2}$$

Collecting terms in the above equation gives

$$(\Delta A)^2 = \frac{1}{\Omega^2} \sum_{i,j} \sum_{\vec{m},\vec{k}}{}' -(\vec{k}\cdot\vec{m}) \phi(k) \phi(m) e^{i\vec{k}\cdot\vec{r}_i} e^{-i\vec{m}\cdot\vec{r}_j} \sum_{a} e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a}. \tag{3.3}$$

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We are now in a position to apply the random phase approximation (see Appendix D) to Eq. (3.3). This approximation replaces $\sum_a e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a}$ by $N\delta_{\vec{k},-\vec{m}}$ with the result that

$$(\Delta A)^2 \cong \frac{1}{\Omega^2} \sum_{i,j} \sum_{\vec{k},\vec{m}}' -(\vec{k}\cdot\vec{m})\phi(k)\phi(m)e^{-i\vec{k}\cdot\vec{r}_i}e^{-i\vec{m}\cdot\vec{r}_j}(N\delta_{\vec{k},-\vec{m}}), \quad (3.4)$$

where $\delta_{\vec{k},-\vec{m}}$ is the Kronecker delta symbol. Summing over $\vec{m}$ gives

$$(\Delta A)^2 \cong \frac{N}{\Omega^2} \sum_{i,j} \sum_{\vec{k}}' k^2\phi^2(k)e^{i\vec{k}\cdot\vec{r}_{ij}}. \quad (3.5)$$

In order to simplify the notation in the following development, let us now define the term in Eq. (2.25) which contains $(\Delta A)^2$ in the following manner:

$$I \equiv \frac{\hbar^2}{8mQ}\int (\Delta A)^2\Psi^*\Psi d\tau, \quad (3.6)$$

where $Q = \int \Psi^*\Psi d\tau$. Combining Eq. (3.5) with Eq. (3.6) leads to the conclusion that

$$I \cong \frac{\hbar^2\rho}{8mQ}\int\left|\rho\sum_{\vec{k}}' k^2\phi^2(k)+\frac{1}{\Omega}\sum_{i\neq j}\sum_{\vec{k}}' k^2\phi^2(k)e^{i\vec{k}\cdot\vec{r}_{ij}}\right|\Psi^*\Psi d\tau. \quad (3.7)$$

From the footnote to Eq. (1.2) we see that

$$\phi(k) = \frac{4\pi ab^2}{k^2(k^2+b^2)}. \quad (3.8)$$

Substituting Eq. (3.8) into Eq. (3.7) gives

$$I = \frac{\hbar^2\rho}{8mQ}(4\pi ab^2)^2\int\left|\rho\sum_{\vec{k}}' \frac{1}{k^2(k^2+b^2)^2}+\frac{1}{\Omega}\sum_{i\neq j}\sum_{\vec{k}}' \frac{e^{i\vec{k}\cdot\vec{r}_{ij}}}{k^2(k^2+b^2)^2}\right|\Psi^*\Psi d\tau. \quad (3.9)$$

The first term is easily evaluated. Replacing the summation sign by its corresponding integral and performing the integration yields

$$\frac{\hbar^2\rho^2}{8m}(4\pi ab^2)^2 \sum_{\vec{k}}{}' \frac{1}{k^2(k^2+b^2)^2} = N\frac{\hbar^2\rho}{8m}(2\pi)^{-3}\int \frac{d\vec{k}}{k^2(k^2+b^2)^2} = N\frac{a^2b}{6\pi}\,\varepsilon_F. \quad (3.10)$$

From symmetry and the definition of $g(r)$, as given by Eq.(1.6), we

see that the second term of Eq.(3.9) may be written as

$$\frac{\hbar^2\rho}{8m}(4\pi ab^2)^2 \frac{\sum_{i\neq j}\int \left|\frac{1}{\Omega}\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{r}_{ij}}}{k^2(k^2+b^2)^2}\right|\Psi^*\Psi d\tau}{\int\Psi^*\Psi d\tau}$$

$$(3.11)$$

$$= \frac{\hbar^2\rho^3}{8m}(4\pi ab^2)^2 \int \left|\frac{1}{\Omega}\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2}\right|g(r_{12})d\vec{r}_1 d\vec{r}_2.$$

We now treat the right hand side of Eq.(3.11) in the same manner as

the potential energy term of Chapter II. To this end, consider the

following development:

$$\int \int \left|\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2}\right|d\vec{r}_1 d\vec{r}_2$$

$$= \sum_{\vec{k}}{}'\frac{1}{k^2(k^2+b^2)^2}\int e^{i\vec{k}\cdot\vec{r}_{12}}d\vec{r}_1 d\vec{r}_2 \qquad (3.12)$$

$$= \Omega^2\sum_{\vec{k}}{}'\frac{1}{k^2(k^2+b^2)^2}\,\delta(\vec{k})\delta(-\vec{k}) = 0.$$

Therefore

$$\int \int \left|\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2}\right|g(r_{12})d\vec{r}_1 d\vec{r}_2$$

$$(3.13)$$

$$= \int \int \left|\sum_{\vec{k}}{}'\frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2}\right|[g(r_{12})-1]d\vec{r}_1 d\vec{r}_2.$$

Integrating over the summation in Eq.(3.13) yields

$$\frac{1}{\Omega} \sum_{\vec{k}}{}' \frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2} = (2\pi)^{-3} \frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{k^2(k^2+b^2)^2} d\vec{k}$$

$$= \frac{1}{8\pi b^4 r}[2-(2+br)e^{-br}]. \qquad (3.14)$$

Applying the results obtained in Eq.(3.13) and Eq.(3.14) to the right hand side of Eq.(3.11), we find

$$\frac{\hbar^2\rho^3}{8m}(4\pi ab^2)^2 \left| \left|\frac{1}{\Omega} \sum_{\vec{k}}{}' \frac{1}{k^2(k^2+b^2)^2}\right| g(r_{12})d\vec{r}_1 d\vec{r}_2 \right.$$

$$= \frac{\hbar^2\rho}{2m} \left(\frac{2a^2}{36\pi^2}\right) \int \frac{[2-(2+br_{12})e^{-br_{12}}]}{r_{12}}[g(r_{12})-1]d\vec{r}_1 d\vec{r}_2. \qquad (3.15)$$

Integrating over the coordinates of particle 1 and changing to Fermi units (see Appendix B), shows that the right hand side of this equation equals

$$N\varepsilon_F\left(\frac{2a^2}{9\pi^2}\right) \int [2-(2+br)e^{-br}][g(r)-1]rdr. \qquad (3.16)$$

Using the above result, along with that obtained in Eq.(3.10), in Eq.(3.9) we obtain the desired expression for I:

$$I \overset{\sim}{=} N\varepsilon_F \left| \frac{a^2b}{6\pi} + \frac{2a^2}{9\pi^2} \int [2-(2+br)e^{-br}][g(r)-1]rdr \right|. \qquad (3.17)$$

Substituting Eq.(3.17) into Eq.(2.28), and converting to Fermi units, gives

$$\frac{<E>_{R.P.}}{N\varepsilon_F} = \frac{3}{5} + \frac{a^2b}{6\pi}$$

$$+ \left(\frac{2a^2}{9\pi^2}\right) \int [2-(2+br)e^{-br}][g(r)-1]rdr \qquad (3.18)$$

$$+ \frac{\gamma^2}{4} \int [g(r)-1]rdr,$$

where

$$\gamma^2 \equiv \frac{8e^2 k_F}{3\pi\varepsilon_F}. \tag{3.19}$$

For purposes which will become apparent in the next chapter, we will

wish to cast Eq. (3.18) in a form which separates out a special term

involving the ideal gas radial distribution function. This special

term, symbolized by e_x, is called the exchange energy, and is defined

by

$$e_x = \frac{\gamma^4}{4}\int [g_I(r)-1]r dr, \tag{3.20}$$

where $g_I(r)$ represents the radial distribution function of the ideal

gas whose wave function is D. Performing the separation we find that

Eq. (3.18) may be rewritten as

$$\frac{<E>_{R.P.}}{N\varepsilon_F} = \frac{3}{5} + \frac{\gamma^2}{4}\int [g_I(r)-1]r dr + \frac{a^2 b}{6\pi}$$

$$+ \frac{2a^2}{9\pi^2}\int [2-(2+br)e^{-br}][g(r)-1]r dr \tag{3.21}$$

$$+ \frac{\gamma^2}{4}\int [g(r)-g_I(r)]r dr.$$

The Superposition Approximation

The expression for the energy given in Eq. (2.32) involves a term

containing the function $g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3)$. For convenience, we shall label

the integral expression in this term by

$$L = \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3) d\vec{r}_{12} d\vec{r}_{13}. \tag{3.22}$$

The superposition approximation merely replaces the function $g_3(\vec{r}_1,\vec{r}_2,\vec{r}_3)$

by the product $g(r_{12})g(r_{13})g(r_{23})$. Performing this substitution in Eq.(3.22) yields

$$L \overset{\sim}{=} \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) g(r_{12}) g(r_{13}) g(r_{23}) dr_{12} dr_{13}. \qquad (3.23)$$

By integrating over angles first, it is easy to see that

$$\int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) g(r_{12}) g(r_{13}) d\vec{r}_{12} d\vec{r}_{13} = 0. \qquad (3.24)$$

Thus, Eq.(3.23) may be written as

$$L \overset{\sim}{=} \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) g(r_{12}) g(r_{13}) [g(r_{23})-1] d\vec{r}_{12} d\vec{r}_{13}. \qquad (3.25)$$

In order to uncouple the variables in Eq.(3.25), we now introduce a delta function as follows:

$$L \overset{\sim}{=} \int \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) g(r_{12}) g(r_{13}) [g(r_{23})-1]$$

$$(3.26)$$

$$\delta(\vec{r}_{23} - \vec{r}_{13} + \vec{r}_{12}) d\vec{r}_{12} d\vec{r}_{13} d\vec{r}_{23}.$$

Noting that

$$\delta(r) = (2\pi)^{-3} \int e^{i\vec{k} \cdot \vec{r}} d\vec{k}, \qquad (3.27)$$

we see that Eq.(3.26) can be written as

$$L \overset{\sim}{=} (2\pi)^{-3} \int_{\vec{k}} d\vec{k} \left\{ \left| \int \nabla_1 u(r_{12}) g(r_{12}) e^{i\vec{k} \cdot \vec{r}_{12}} dr_{12} \right. \right.$$

$$(3.28)$$

$$\left. \cdot \int \nabla_1 u(r_{13}) g(r_{13}) e^{-i\vec{k} \cdot \vec{r}_{13}} dr_{13} \right| \left| \int (g(r_{23})-1) e^{i\vec{k} \cdot \vec{r}_{23}} dr_{23} \right| \right\}.$$

The integrals involving the gradients are evaluated as follows:

$$\int \nabla_1 u(r_{12}) g(r_{12}) e^{i\vec{k} \cdot \vec{r}_{12}} dr_{12} = \int \hat{r}_{12} \frac{du(r_{12})}{dr_{12}} g(r_{12}) e^{i\vec{k} \cdot \vec{r}_{12}} dr_{12}, \qquad (3.29)$$

where $\hat{r}_{12}$ is a unit vector in the direction of $\vec{r}_{12}$. Taking $\vec{k}$ in the azimuthal direction and carrying out the integration over angles yields

$$\int \hat{r}_{12} \frac{du(r_{12})}{dr_{12}} g(r_{12}) e^{i\vec{k}\cdot\vec{r}_{12}} dr_{12}$$

$$= \hat{i}_k (2\pi) \int \frac{du(r_{12})}{dr_{12}} g(r_{12}) e^{ikr_{12}\cos\theta} r_{12}^2 \sin\theta \cos\theta \, d\theta \, dr_{12} \qquad (3.30)$$

$$= \hat{i}_k (4\pi i) \int \frac{du(r_{12})}{dr_{12}} g(r_{12}) r_{12}^2 \left| \frac{\cos kr_{12}}{kr_{12}} - \frac{\sin kr_{12}}{k^2 r_{12}^2} \right| dr_{12},$$

where $\hat{i}_k$ is a unit vector in the $\vec{k}$ direction. The integral involving $\vec{r}_{13}$ is just the complex conjugate of this expression with r_{13} replacing r_{12}.

Substituting the above results into Eq.(3.28) shows that

$$L \cong \frac{2}{\pi} \int\limits_{\vec{k}} d\vec{k} \left| \int (g(s)-1) e^{i\vec{k}\cdot\vec{s}} ds \right|$$

$$\left| \int \left(\frac{\cos kr}{kr} - \frac{\sin kr}{k^2 r^2} \right) \frac{du(r)}{dr} g(r) r^2 dr \right|^2, \qquad (3.31)$$

where $\vec{r}_{23} \equiv \vec{s}$, and $\vec{r} \equiv \vec{r}_{12} = \vec{r}_{13}$.

Noting the fact that

$$\frac{d}{dk} \left(\frac{\sin kr}{kr^2} \right) = \frac{\cos kr}{kr} - \frac{\sin kr}{k^2 r^2},$$

and taking the derivative of $u(r)$, we find that Eq.(3.31) may be written as

$$L \cong \frac{2}{\pi} \int\limits_{\vec{k}} d\vec{k} \left| \int (g(s)-1) e^{i\vec{k}\cdot\vec{s}} ds \right| \left| \left\{ \frac{d}{dk} \right\} \right| be^{-br}$$

$$- \frac{(1-e^{-br})}{r} \left| \frac{\sin kr}{kr^2} \frac{g(r)}{r} r^2 dr \right\}^2. \qquad (3.32)$$

Finally, from Eq.(3.32) it is apparent that the expression for L may be written in terms of Fourier transforms as follows:

$$L \overset{\simeq}{=} (2\pi)^{-3} \int_{\vec{k}} d\vec{k} \left| \int (g(s)-1) e^{i\vec{k}\cdot\vec{s}} d\vec{s} \right| \left\{ \frac{d}{dk} \int \left| be^{-br} - \frac{(1-e^{-br})}{r} \right| \frac{g(r)}{r^2} e^{i\vec{k}\cdot\vec{r}} d\vec{r} \right\}^2 . \quad (3.33)$$

Using this equation, along with the derivative of u(r), in Eq.(2.32) we find that, for the superposition approximation

$$\frac{<E>_s}{N\epsilon_F} = \frac{3}{5} + \frac{a^2}{3\pi} \int \left| \frac{1-2e^{-br}+e^{-2br}}{r^2} - \frac{2b(e^{-br}-e^{-2br})}{r} + b^2 e^{-2br} \right| g(r) dr$$

$$+ \frac{1}{288\pi^7} \int_{\vec{k}} d\vec{k} \left| \int (g(s)-1) e^{i\vec{k}\cdot\vec{s}} d\vec{s} \right| \left\{ \frac{d}{dk} \int \left| be^{-br} - \frac{(1-e^{-br})}{r} \right| \right. \quad (3.34)$$

$$\left. \frac{g(r)}{r^2} e^{i\vec{k}\cdot\vec{r}} d\vec{r} \right\}^2 + \frac{\gamma^2}{4} \int [g(r)-1] r dr,$$

where Fermi units are again employed. Following the procedure adopted in the first section of this chapter, we now rewrite Eq.(3.34) in terms of the exchange energy. Doing this yields

$$\frac{<E>_s}{N\epsilon_F} = \frac{3}{5} + \frac{\gamma^2}{4} \int [g_I(r)-1] r dr$$

$$+ \frac{a^2}{3\pi} \int \left| \frac{1-2e^{-br}+e^{-2br}}{r^2} - \frac{2b(e^{-br}-e^{-2br})}{r} + b^2 e^{-2br} \right| g(r) dr$$

$$+ \frac{1}{288\pi^7} \int_{\vec{k}} d\vec{k} \left| \int (g(s)-1) e^{i\vec{k}\cdot\vec{s}} d\vec{s} \right| \left\{ \frac{d}{dk} \int \left| be^{-br} - \frac{(1-e^{-br})}{r} \right| \right. \quad (3.35)$$

$$\left. \frac{g(r)}{r} e^{i\vec{k}\cdot\vec{r}} d\vec{r} \right\}^2 + \frac{\gamma^2}{4} \int [g(r)-g_I(r)] r dr.$$

Variational Techniques

So far, it has been the purpose of this work to reduce the energy expression, given by Eq.(1.5), to a suitable form depending on the two unknown parameters a and b. This having been done

in Eq. (3.21) and Eq. (3.35), we now proceed to the actual variational

techniques[10] employed in calculating the ground state energies, and

their corresponding wave functions, for various densities. It is

apparent, upon consideration of Eq. (3.21) and Eq. (3.35), that the

last three terms of each of these equations are the only terms con-

taining the unknowns a and b. The sum of these terms is called the

correlation energy and is symbolized by the expression e_c. Since

the first two terms of the final energy equations do not depend on

a and b, the minimum value of the energy with respect to the two

parameters can be found by minimizing e_c alone. The variational

principle tells us that, if we arbitrarily vary a and b and find a

combination of these two numbers which gives us the lowest value for

e_c, then this value is the best approximation to the ground state

correlation energy for the originally adopted form of u(r). The

variation of a and b is carried out as follows:

(1) Fix b at some convenient value, and compute e_c for several

values of a. This procedure will yield one particular value of a,

which we shall call a_1, corresponding to a local minimum in the

value of e_c. An example of this, for a particular density, is given

in Fig. 1.

(2) Having found a_1, we now compute e_c for various different

b values, holding a fixed at the value obtained in step 1. This

gives a value for b, called b_1, at which e_c is again found to be

a minimum (see Fig. 2).

(3) Fixing b at the value b_1 we now vary a again, searching

for a still lower minimum in the neighborhood of a_1.

This process is carried on until reasonable accuracy is obtained.
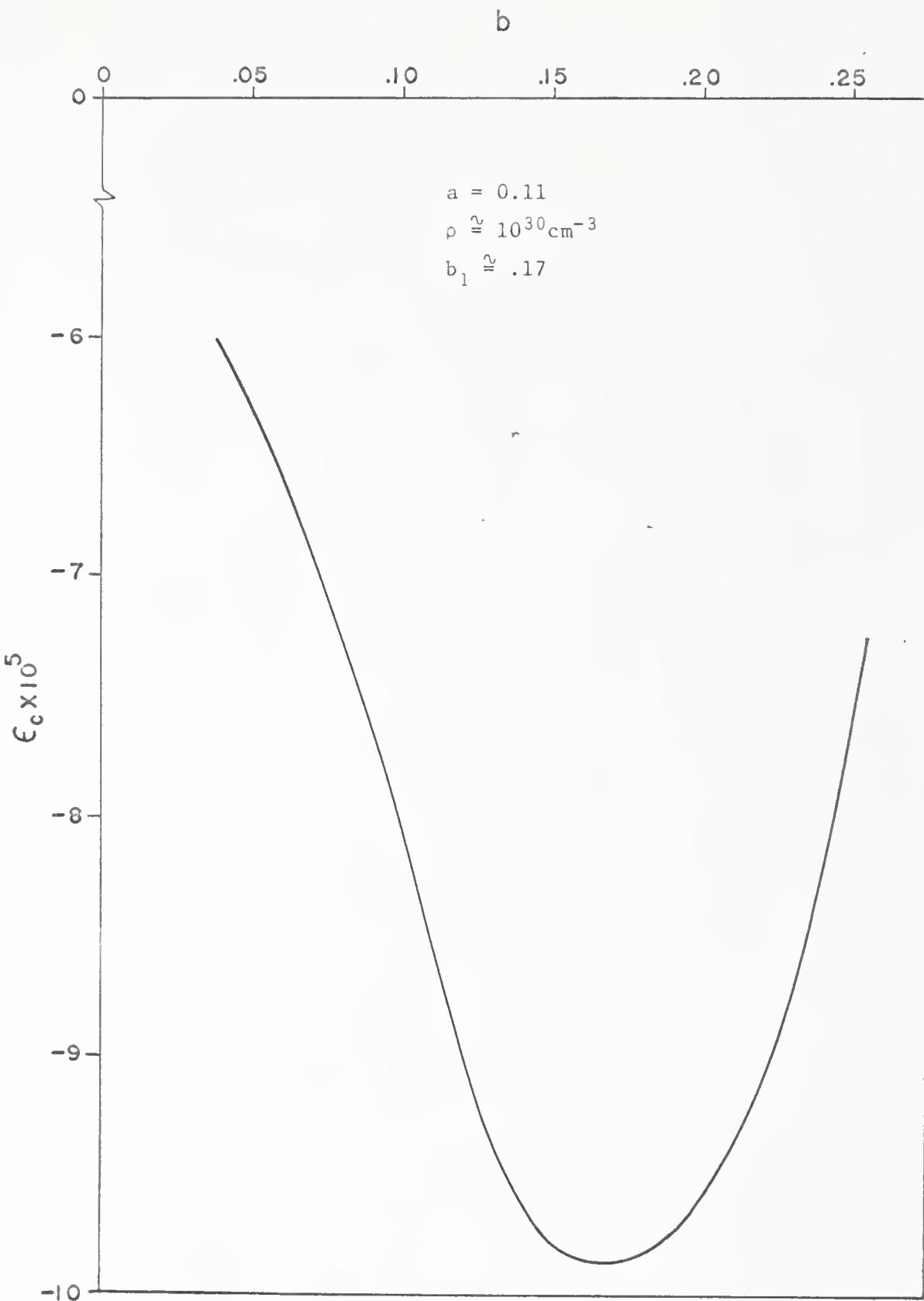
Fig. 1. Variation of the First Parameter.
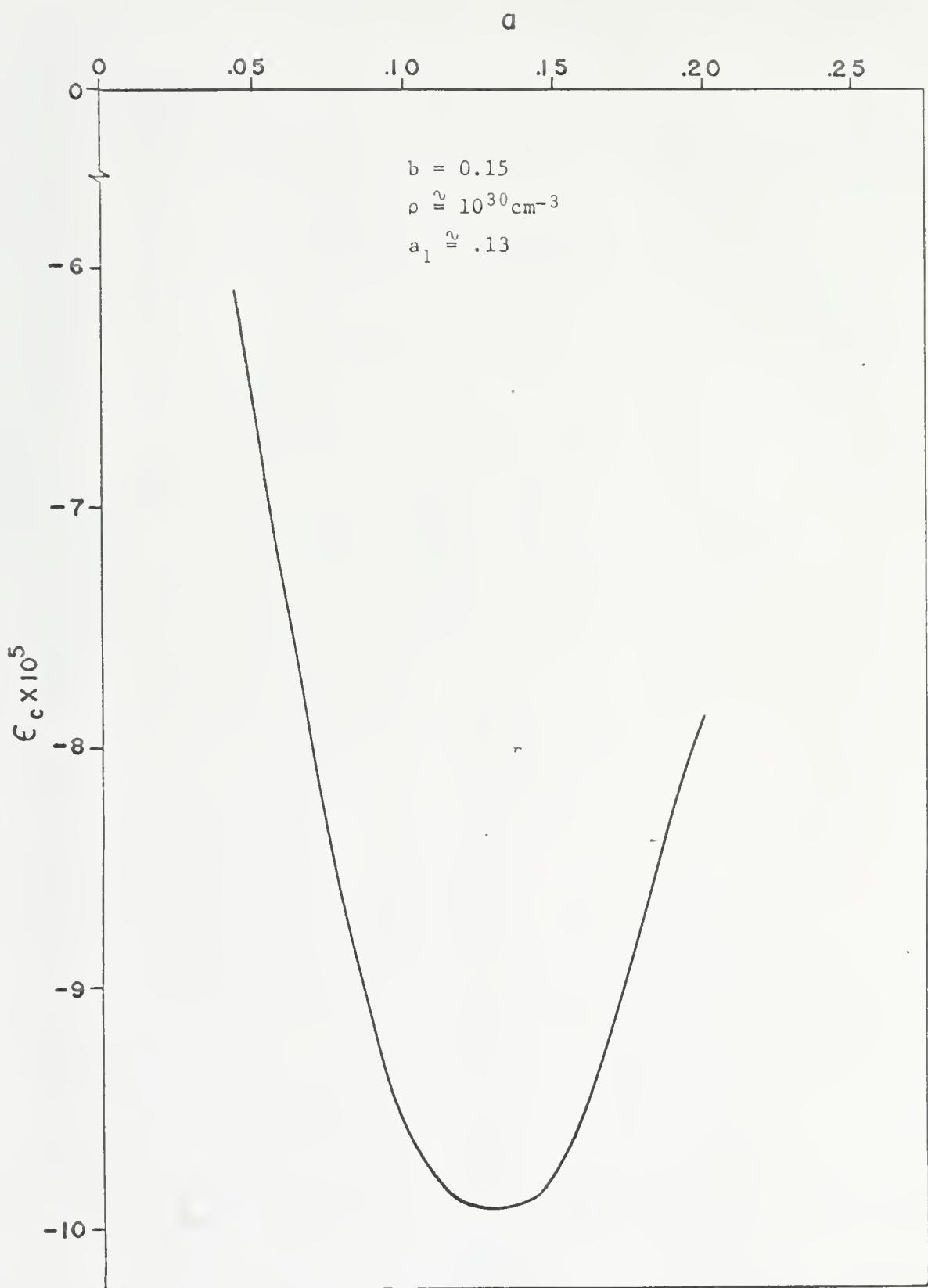
Fig. 2. Variation of the Second Parameter.

CHAPTER IV

DISCUSSION AND RESULTS

Before presenting the results of the calculations described in
Chapter III, a brief summary of the approximations used to obtain
those results is in order.   The approximations are:

(1) It is assumed that the wave function Ψ can be expressed as

$$\Psi = D\exp[-\frac{1}{2}\sum_{i<j} u(r_{ij})],$$

where D is the wave function for an ideal gas of spin 1/2 particles.

(2) $$|D|^2 = \exp[-\sum_{i<j} \phi(r_{ij})].[3]$$

(3) It is assumed that the effective potential $u(r)$ can be
written as

$$u(r) = \frac{a}{r}(1-e^{-br}),$$

where a and b are parameters to be determined.

(4) The energy expressions are simplified by the application
of either a random phase approximation[1,13] or a superposition ap-
proximation.[9,10]

(5) The radial distribution function $g(r)$ is computed by use
of either the Percus-Yevick integral equation[5] or the Lado pertur-
bation formula.[4,11]

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The numerical results of the energy calculations are given in the table below. Graphs, and other pertinent information, can be found in Appendix E. The notation employed in Table 1 is the following:

r_s = the ion sphere radius in Bohr units.

$\gamma^2 = 1.13 r_s$.

$E_{R.P.A./L.}$ = the minimum correlation energy found by using the random phase approximation and the Lado perturbation formula.

$E_{S.A./P.-Y.}$ = the minimum correlation energy found by using the superposition approximation and the Percus-Yevick integral equation.

$E_{S.A./L.}$ = the minimum correlation energy found by using the superposition approximation and the Lado perturbation formula.

TABLE 1

The Ground State Correlation Energies

r_s	γ^2	$E_{R.P.A./L.}$	$E_{S.A./L.}$	$E_{S.A./P.-Y.}$
.00113	.001	−.00000012	−	−
.0113	.01	−.000010	−	−
.113	.1	−.00053	−.00047	−
1.13	1.0	−.019	−.018	−.039
3.39	3.0	−	−	−.29
5.65	5.0	−	−	−.65

The accurate calculation of the correlation energies listed in Table 1 is a somewhat delicate task. This is particularly true in the region of intermediate densities. The difficulties encountered are largely the consequence of cancellation among the various terms which make up the correlation energy expression. Using the definition of e_c given in the last section of Chapter III, along with Eq. (3.35), we see that the correlation energy may be written as

$$\varepsilon_c = \varepsilon_1 + \varepsilon_2 + \varepsilon_3,$$

where

$$\varepsilon_1 = \frac{a^2}{3\pi}\int\left|\frac{(1-e^{-br})}{r^2} - 2b\frac{(e^{-br}-e^{-2br})}{r} + b^2e^{-2br}\right|g(r)dr,$$

$$\varepsilon_2 = \frac{1}{288\pi^7}\int d\vec{k}\left\{\int [g(s)-1]e^{i\vec{k}\cdot\vec{s}}d\vec{s}\right\}\left\{\frac{d}{dk}\int\left|be^{-br}-\frac{(1-e^{-br})}{r}\right|\frac{g(r)}{r^2}e^{i\vec{k}\cdot\vec{r}}d\vec{r}\right\}^2,$$

and

$$\varepsilon_3 = \frac{\gamma^2}{4}\int [g(r)-g_I(r)]rdr.$$

Adopting this notation in Table 3 we are able to observe the cancellation referred to above.

TABLE 2

Cancellation in the Intermediate Region

γ^2	ε_1	ε_2	ε_3	ε_c
1.0	+.118	-.078	-.079	-.039
3.0	+.897	-.690	-.498	-.291
5.0	+1.34	-1.05	-.940	-.653

A comparison between the results of the variational method used
in this work, and the results of some other approaches is given below
in Table 4.

TABLE 3

Comparison of Ground State Energies

γ^2	Variational method (Parametric)	High Density Expansion[*]	Wigner[†]	Dunn[††]
.001	−.00000012	−.00000018	−	−.00000057
.01	−.000010	−.000013	−	−.000026
.1	−.00053	−.00084	−	−.0011
1.0	−.039	−.043	−.034	−.051
3.0	−.29	−	−.24	−.30
5.0	−.65	−	−.568	−.624

[*]W. J. Carr, Jr., Phys. Rev. 133, A371 (1964).

[†]F. Wigner, Trans. Faraday Soc. 34, 678 (1938).

[††]T. Dunn, dissertation, University of Florida (1966); Tucson Dunn
and A. A. Broyles, Phys. Rev. 157, 156 (1967).

The above table seems to imply that the parametric method is
giving reasonably accurate results over a wide range of densities,
including the region of metallic densities. This was the hoped-for
result. Another suggestive feature of these calculations concerns
the nature of the radial distribution function. Several methods of
calculating this function, for a given effective potential, utilize

an approximation which considers the contribution of the "bridge dia-grams"[4,14] in a cluster expansion of $g(r)$ to be negligible. The cal-culations done in this dissertation, along with those of T. Dunn, contain that approximation, while those of Carr and Wigner do not. The observed agreement between the results obtained by these different approaches seems to indicate that the above assumption concerning the "bridge diagrams" is a good approximation.

Finally, it must be noted that the parametric form chosen for the effective potential in this work can only be expected to yield a good approximation to the true answer. In order to determine the exact form for the effective potential, one must apply a rigorous variational procedure to the expression for the energy given by Eq.(2.32). This process would yield an integro-differential equa-tion involving the effective potential and the radial distribution function. The derivation of such an equation is now in progress, and it is hoped that the results of this dissertation will provide the initial information necessary to solve it.

APPENDIX A

THE ELECTRON GAS

The electron gas is defined as a system of N electrons in a cube of edge length L, and volume $\Omega = L^3$. It is assumed that when N and Ω are large enough, the surface effects are negligible, even though periodic boundary conditions are imposed upon the wave function Ψ. The number of particles and the volume are assumed to be infinite in such a way that the density $\rho = \frac{N}{\Omega}$, remains finite.

In order that the total charge of the system remains neutral, we assume that the electrons move in a uniform positive background whose total charge just cancels that of the electrons. Each electron has associated with it an "ion sphere" whose radius is given by

$$r_o = \left(\frac{4}{3\pi\rho}\right)^{1/3}. \tag{A.1}$$

We now write the density $\rho(\vec{r})$ as[1]

$$\rho(\vec{r}) = \rho_e(\vec{r}) + \bar{\rho}, \tag{A.2}$$

where $\rho_e(\vec{r})$ is the electron density, and $\bar{\rho}$ is the density of the uniform positive background. Using Eq.(A.2), we see that the potential energy for the system may be written as

$$U = \frac{e^2}{2} \int \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r}-\vec{r}!|} \, d\vec{r}d\vec{r}'$$

$$= \frac{e^2}{2} \left\{ \int \frac{\rho_e(\vec{r})\rho_e(\vec{r}')}{|\vec{r}-\vec{r}'|} \, d\vec{r}d\vec{r}' - 2\bar{\rho}\int \frac{\rho_e(\vec{r})}{|\vec{r}-\vec{r}'|} \, d\vec{r}d\vec{r}' + \bar{\rho}^2 \int \frac{d\vec{r}d\vec{r}'}{|\vec{r}-\vec{r}'|} \right\}. \tag{A.3}$$

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Since the uniform positive background assured us of charge neutrality, the average electron charge density must be equal to that of the positive background. Using this fact in Eq.(A.3), we see that partial cancellation occurs in the last two terms to yield

$$U = \frac{e^2}{2} \int \frac{\rho_e(\vec{r})\rho_e(\vec{r}')}{|\vec{r}-\vec{r}'|} \, d\vec{r}d\vec{r}'$$

$$- \frac{e^2}{2} \bar{\rho} \int \frac{\rho_e(\vec{r})}{|\vec{r}-\vec{r}'|} \, d\vec{r}d\vec{r}'.$$

(A.4)

It can further be shown[6] that Eq.(A.4) may be written as

$$U = \frac{1}{2\Omega} \sum_{i,j} \sum_{k}' \nu_k e^{i\vec{k}\cdot\vec{r}_{ij}},$$

(A.5)

where

$$\nu_k = \frac{4\pi e^2}{k^2}.$$

APPENDIX B

FERMI UNITS

Fermi units are based on the definition of the Fermi energy given by

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m},$$

where

$$k_F = (3\pi^2 \rho)^{1/3}.$$

The unit of length in these units is

$$a_F = \frac{1}{k_F}.$$

There are two more important quantities used in this work. Expressed in Fermi units they are:

1. The density – $\rho = \dfrac{1}{3\pi^2}$.
2. The density parameter – $\gamma^2 = \dfrac{8e^2 k_F}{3\pi \varepsilon_F}$.

In order that the variables of integration in this paper be dimensionless, the following transformations are made:

$$\vec{r} = \frac{\vec{R}}{k_F}$$

and

$$\vec{k} = k_F \vec{x}.$$

APPENDIX C

IDEAL GAS WAVE FUNCTION

We define the ideal gas wave function as follows:

$$D = \sum_p \epsilon_p e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j} S \qquad (C.1)$$

where S accounts for spin, p is the permutation operator, and ϵ_p is given by

$$\epsilon_p = \begin{cases} +1 \text{ for even permutations} \\ -1 \text{ for odd permutations.} \end{cases}$$

From Eq.(1.4) and the above definition of D we see that

$$\Delta^2 D = \sum_{j=1}^N \nabla_j^2 \left| \sum_p \epsilon_p e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j} S \right|. \qquad (C.2)$$

Taking the gradients gives

$$\Delta^2 D = \sum_{j=1}^N \sum_p \epsilon_p (-\vec{k}_{pj}^2) e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j} S. \qquad (C.3)$$

But,

$$\sum_{j=1}^N \sum_p \epsilon_p (-\vec{k}_{pj}^2) e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j} = \left(-\sum_j \vec{k}_j^2\right) \sum_p \epsilon_p e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j}. \qquad (C.4)$$

Therefore,

$$\Delta^2 D = \left(-\sum_j \vec{k}_j^2\right) \sum_p \epsilon_p e^{i\sum_j^N \vec{k}_{pj} \cdot \vec{r}_j} S$$

$$\qquad (C.5)$$

$$= \left(-\sum_j \vec{k}_j^2\right) D.$$

APPENDIX D

RANDOM PHASE APPROXIMATION

Consider the expression

$$M = \sum_{i,j} e^{i\vec{k}\cdot\vec{r}_i - i\vec{m}\cdot\vec{r}_j} \sum_a e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a}. \qquad (D.1)$$

Averaging over the position of particle a gives

$$M = \sum_{i,j} e^{i\vec{k}\cdot\vec{r}_i} e^{-i\vec{m}\cdot\vec{r}_j} \frac{\rho\Omega^3 \int e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a} \psi^* \psi d\tau'}{\int \psi^* \psi d\tau}, \qquad (D.2)$$

where

$$d\tau' = d\vec{r}_1 \ldots d\vec{r}_{i-1} d\vec{r}_{i+1} \ldots d\vec{r}_{j-1} d\vec{r}_{j+1} \ldots d\vec{r}_N.$$

From the definition of $g_3(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ given by Eq.(2.29) we see that Eq.(D.2) may be written as

$$M = \sum_{i,j} e^{i\vec{k}\cdot\vec{r}_i} e^{-i\vec{m}\cdot\vec{r}_j} (\rho) \int e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a} g_3(\vec{r}_a, \vec{r}_i, \vec{r}_j) d\vec{r}_a. \qquad (D.3)$$

The random phase approximation assumes that the particles are uniformly distributed at random. We can apply this hypothesis to Eq.(D.3) by setting $g_3(\vec{r}_a, \vec{r}_i, \vec{r}_j)$ equal to 1. This yields

$$M \simeq \sum_{i,j} e^{i\vec{k}\cdot\vec{r}_i} e^{-i\vec{m}\cdot\vec{r}_j} \rho \int e^{i(\vec{k}+\vec{m})} d\vec{r}_a. \qquad (D.4)$$

Noting that

$$\Omega^{-1} \int e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a} d\vec{r}_a = \delta_{\vec{k}, -\vec{m}}, \qquad (D.5)$$

we see that Eq.(D.4) becomes

$$M \simeq \sum_{i,j}^{N} e^{i\vec{k}\cdot\vec{r}_i} e^{-i\vec{m}\cdot\vec{r}_j} (N\delta_{\vec{k},-\vec{m}}). \tag{D.6}$$

Taking a different view of the problem, we might have considered the term $\sum_a^{N} e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a}$ alone. The theory of "Random Walk" tells us that, if $(\vec{k}+\vec{m})$ is not equal to zero, then the summation is equal to $\sqrt{N}$. If, however, $(\vec{r}+\vec{m})$ is equal to zero, then the summation equals N. Since our model allows the number of particles to approach infinity, we see that the $(\vec{k}+\vec{m}) = 0$ term will dominate. Thus

$$\sum_a^{N} e^{i(\vec{k}+\vec{m})\cdot\vec{r}_a} \simeq N\delta_{\vec{k},-\vec{m}}. \tag{D.7}$$

APPENDIX E

NUMERICAL RESULTS FOR THE
VARIATIONAL CALCULATIONS

The following are a series of graphs and tables summarizing the results of the calculations done in this work. The high density curve in Fig. (E.2) comes from the results of Bohm and Pines.[6]

TABLE E.1

The Ground State Radial Distribution Functions

	g(r)					
R	$\gamma^2 = .001$	$\gamma^2 = .01$	$\gamma^2 = .1$	$\gamma^2 = 1.0$	$\gamma^2 = 3.0$	$\gamma^2 = 5.0$
.2	.5039	.5029	.4921	.2130	.0239	.00656
.4	.5157	.5148	.5051	.2531	.0427	.01528
.6	.5349	.5341	.5254	.2989	.0709	.03134
.8	.5606	.5598	.5521	.3487	.1094	.05735
1.0	.5918	.5911	.5841	.4030	.1594	.09598
1.4	.6661	.6655	.6598	.5209	.2926	.1486
1.8	.7470	.7465	.7420	.6432	.4597	.3885
2.2	.8244	.8240	.8205	.7579	.6381	.5894
2.6	.8903	.8900	.8873	.8545	.8011	.7829
3.0	.9402	.9399	.9378	.9270	.9278	.9271
3.4	.9732	.9730	.9713	.9740	1.009	1.035
3.8	.9914	.9912	.9900	.9992	1.047	1.077
4.2	.9988	.9986	.9977	1.009	1.053	1.078
5.2	.9975	.9974	.9969	1.004	1.014	1.011
6.2	.9969	.9968	.9966	.9989	.9908	.9809
7.2	.9996	.9995	.9994	1.000	.9950	.9938
8.2	.9998	.9997	.9997	1.000	1.001	1.005
9.2	.9994	.9993	.9993	.9996	1.001	1.003
10.2	.9998	.9998	.9998	.9999	1.000	.9991

TABLE E.2

The Variational Parameters for Which Minimum
Energies Were Found

γ^2	$a_{R.P.A./L.}$	$a_{S.A./L.}$	$a_{S.A./P.-Y.}$	$b_{R.P.A./L.}$	$b_{S.A./L.}$	$b_{S.A./P.-Y.}$
.001	.025	–	–	.08	–	–
.01	.13	–	–	.17	–	–
.1	.48	.45	–	.28	.3	–
1.0	1.3	–	1.5	.4	–	1.25
3.0	–	–	4.2	–	–	1.4
5.0	–	–	5.3	–	–	1.5

The notation used in the table above is the following:

R.P.A. means random phase approximation.[1,13]

L. means Lado perturbation formula.[4,11]

S.A. means superposition approximation.[9,10]

P.-Y. means Percus-Yevick integral equation.[5]
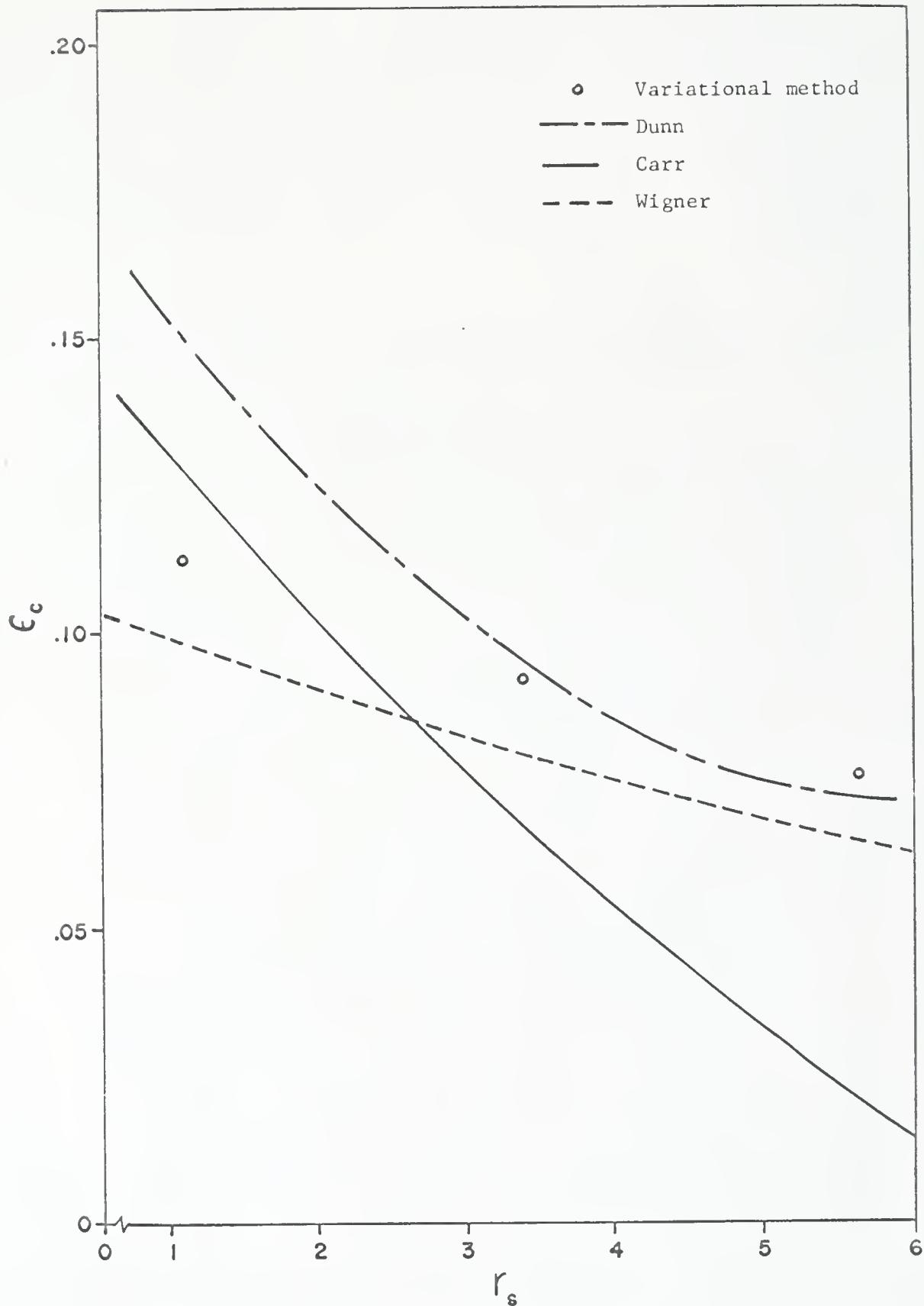
Fig. E.1.   Comparison of Ground State Energies for Intermediate
   Densities.
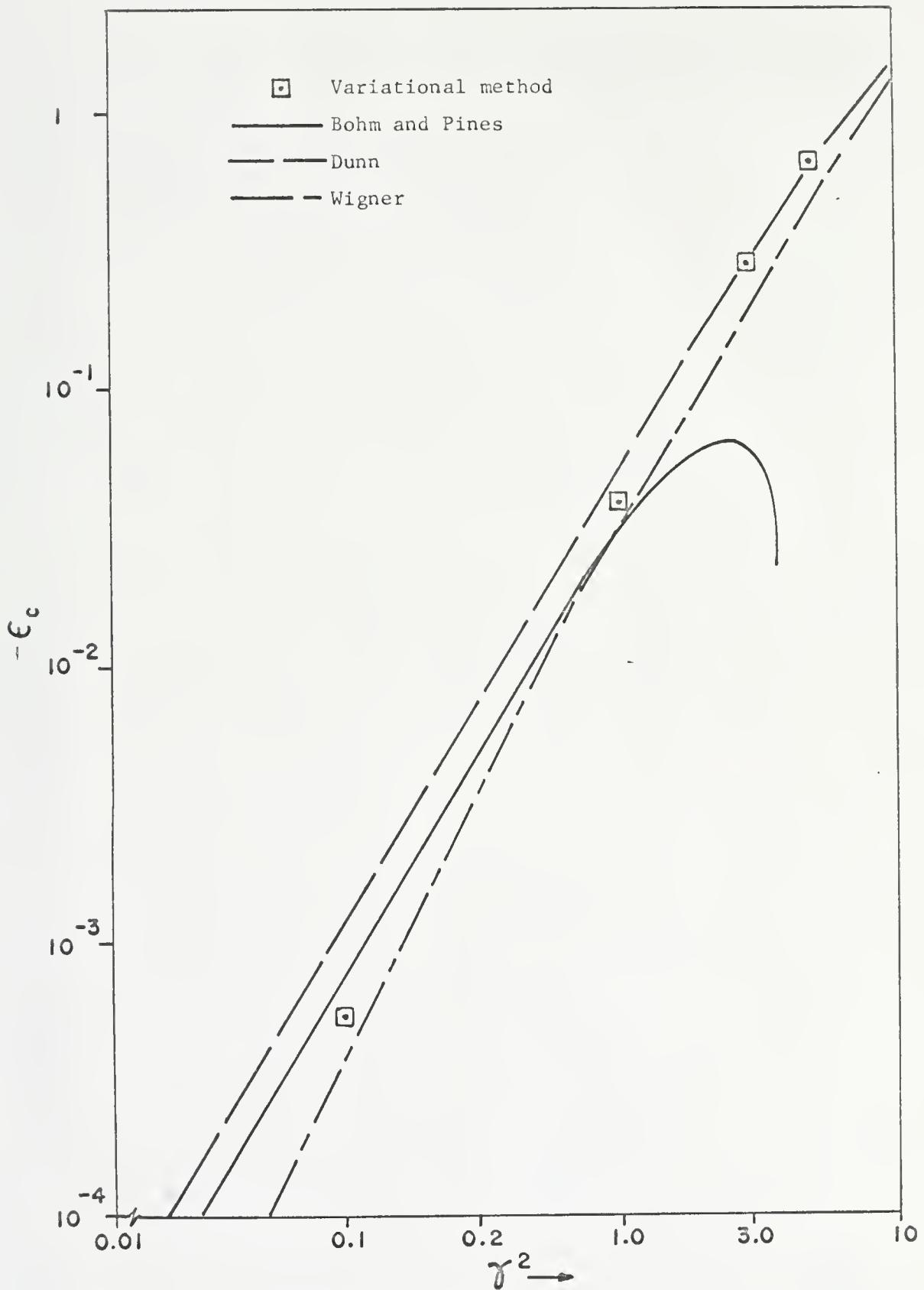
Fig. E.2. Logarithmic Comparison of Ground State Energies.

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This dissertation was prepared under the direction of the chairman of the candidate's supervisory committee and has been approved by all members of that committee. It was submitted to the Dean of the College of Arts and Sciences and to the Graduate Council, and was approved as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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